

chain nodes :

17 18 19 21 29 30 31 32 33 34 35 36 37 38 43 44 51 55 56 59

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 23 24 25 26 27 28 45
46 47 48 49 50

chain bonds :

8-17 10-19 12-17 17-18 29-30 31-32 33-34 34-35 36-37 37-38 43-44 50-51

55-56

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 11-12 11-16 12-13 13-14 14-15 15-16 12-13 13-14
14-15 15-16 23-24 23-28 24-25 25-26 26-27 27-28 45-46 45-50 46-47 47-48 48-49 49-50

exact/norm bonds :

10-19 17-18 29-30 31-32 33-34 34-35 36-37 37-38 43-44 50-51 55-56

exact bonds :

5-7 6-10 7-8 8-9 8-17 9-10 12-17

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-16 12-13 13-14 14-15 15-16 23-24
23-28 24-25 25-26 26-27 27-28 45-46 45-50 46-47 47-48 48-49 49-50

isolated ring systems :

containing 1 : 11 :

G1: [*1], [*2], [*3], [*4], [*5], [*6], [*7], [*8]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:CLASS 19:CLASS
21:CLASS 22:CLASS 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:CLASS
30:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS 35:CLASS 36:CLASS 37:CLASS
38:CLASS 43:CLASS 44:CLASS 45:Atom 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom
51:CLASS 55:CLASS 56:CLASS 59:CLASS Page 3 ASS

L1 STRUCTURE uploaded

=> d

L1 HAS NO ANSWERS

L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s l1 ful

FULL SEARCH INITIATED 12:35:32 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 61 TO ITERATE

100.0% PROCESSED 61 ITERATIONS

SEARCH TIME: 00.00.01

0 ANSWERS

L2 0 SEA SSS FUL L1

=>

---Logging off of STN---

=>

Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

FULL ESTIMATED COST

ENTRY

SESSION

161.76

161.97

STN INTERNATIONAL LOGOFF AT 12:36:16 ON 17 APR' 2005

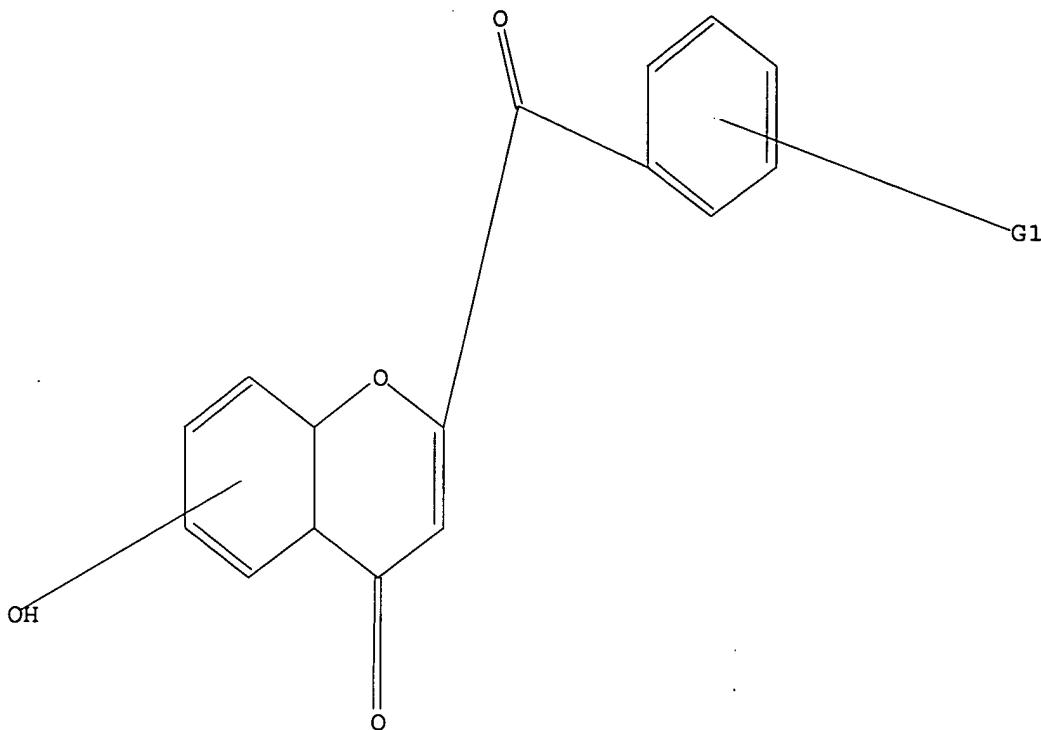
L8 STRUCTURE UPLOADED

10 / 725349

=> d

L8 HAS NO ANSWERS

L8 STR



G1 Cl,Br,F,I,OH,MeO,EtO,n-BuO,COOH,SO2,OSO3H,SO3H,CHO,H

Structure attributes must be viewed using STN Express query preparation.

=> s 18 ful

FULL SEARCH INITIATED 14:23:45 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 5027 TO ITERATE

100.0% PROCESSED 5027 ITERATIONS

12 ANSWERS

SEARCH TIME: 00.00.01

L9 12 SEA SSS FUL L8

=> d 1-12

L9 ANSWER 1 OF 12 REGISTRY COPYRIGHT 2005 ACS on STN

RN 791569-53-4 REGISTRY

ED Entered STN: 02 Dec 2004

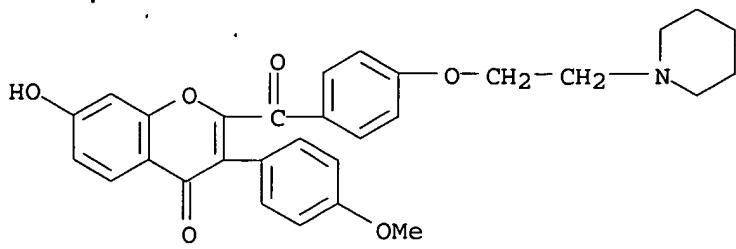
CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-methoxyphenyl)-2-[4-[2-(1-piperidinyl)ethoxy]benzoyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C30 H29 N O6

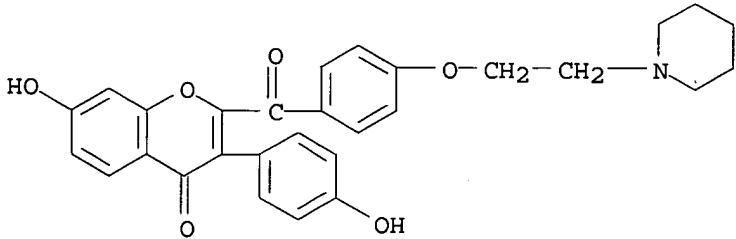
CI COM

SR CA



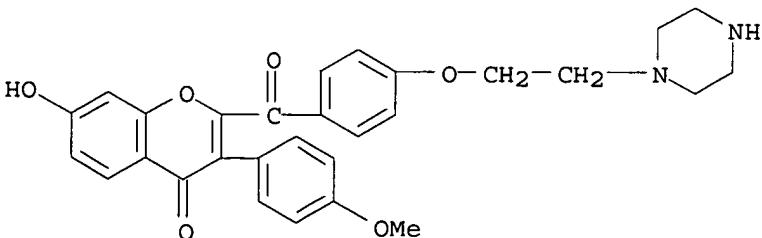
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L9 ANSWER 2 OF 12 REGISTRY COPYRIGHT 2005 ACS on STN
RN 776277-97-5 REGISTRY
ED Entered STN: 08 Nov 2004
CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-hydroxyphenyl)-2-[4-[2-(1-piperidinyl)ethoxy]benzoyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C29 H27 N O6
CI COM
SR CA



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

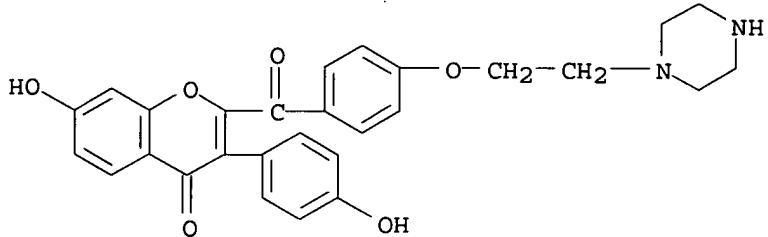
L9 ANSWER 3 OF 12 REGISTRY COPYRIGHT 2005 ACS on STN
RN 748753-01-7 REGISTRY
ED Entered STN: 21 Sep 2004
CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-methoxyphenyl)-2-[4-[2-(1-piperazinyl)ethoxy]benzoyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C29 H28 N2 O6
CI COM
SR CA



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

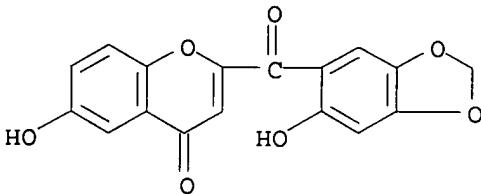
L9 ANSWER 4 OF 12 REGISTRY COPYRIGHT 2005 ACS on STN

RN 721881-00-1 REGISTRY
ED Entered STN: 03 Aug 2004
CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-hydroxyphenyl)-2-[4-[2-(1-piperazinyl)ethoxy]benzoyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C28 H26 N2 O6
CI COM
SR CA



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

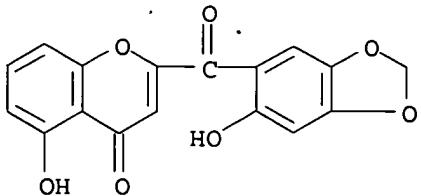
L9 ANSWER 5 OF 12 REGISTRY COPYRIGHT 2005 ACS on STN
RN 700818-30-0 REGISTRY
ED Entered STN: 29 Jun 2004
CN 4H-1-Benzopyran-4-one, 6-hydroxy-2-[(6-hydroxy-1,3-benzodioxol-5-yl)carbonyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H10 O7
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

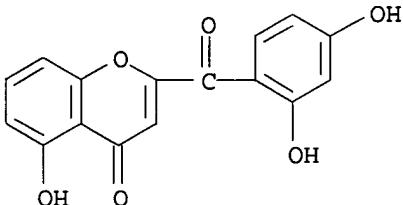
L9 ANSWER 6 OF 12 REGISTRY COPYRIGHT 2005 ACS on STN
RN 700818-27-5 REGISTRY
ED Entered STN: 29 Jun 2004
CN 4H-1-Benzopyran-4-one, 5-hydroxy-2-[(6-hydroxy-1,3-benzodioxol-5-yl)carbonyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H10 O7
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

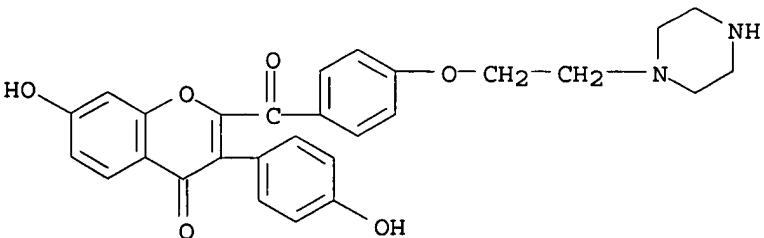
L9 ANSWER 7 OF 12 REGISTRY COPYRIGHT 2005 ACS on STN
RN 700818-24-2 REGISTRY
ED Entered STN: 29 Jun 2004
CN 4H-1-Benzopyran-4-one, 2-(2,4-dihydroxybenzoyl)-5-hydroxy- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C16 H10 O6
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

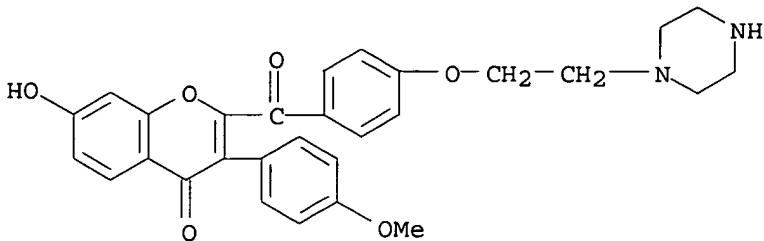
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L9 ANSWER 8 OF 12 REGISTRY COPYRIGHT 2005 ACS on STN
RN 209669-52-3 REGISTRY
ED Entered STN: 09 Aug 1998 ✓
CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-hydroxyphenyl)-2-[4-[(1-piperazinyl)ethoxy]benzoyl]-, dihydrochloride (9CI) (CA INDEX NAME)
OTHER NAMES:
CN CHF 3356.01
MF C28 H26 N2 O6 . 2 Cl H
SR CA
LC STN Files: CA, CAPLUS
CRN (721881-00-1)



1 REFERENCES IN FILE CA (1907 TO DATE)
.1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

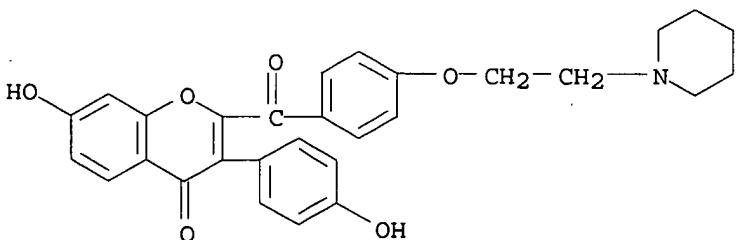
L9 ANSWER 9 OF 12 REGISTRY COPYRIGHT 2005 ACS on STN
RN 209669-51-2 REGISTRY ✓
ED Entered STN: 09 Aug 1998
CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-methoxyphenyl)-2-[4-[2-(1-piperazinyl)ethoxy]benzoyl]-, dihydrochloride (9CI) (CA INDEX NAME)
OTHER NAMES:
CN CHF 3340.01
MF C29 H28 N2 O6 . 2 Cl H
SR CA
LC STN Files: CA, CAPLUS
CRN (748753-01-7)



● 2 HCl

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L9 ANSWER 10 OF 12 REGISTRY COPYRIGHT 2005 ACS on STN
RN 209669-50-1 REGISTRY ✓
ED Entered STN: 09 Aug 1998
CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-hydroxyphenyl)-2-[4-[2-(1-piperidinyl)ethoxy]benzoyl]-, hydrochloride (9CI) (CA INDEX NAME)
OTHER NAMES:
CN CHF 3316.01
MF C29 H27 N O6 . Cl H
SR CA
LC STN Files: CA, CAPLUS
CRN (776277-97-5)

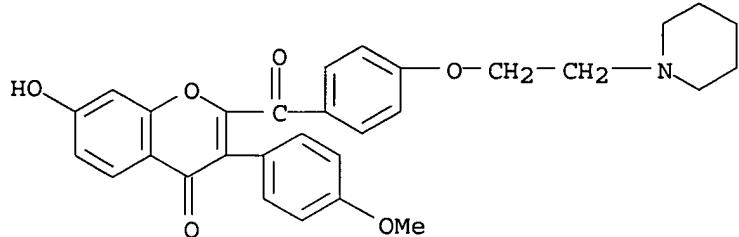


● HCl

1 REFERENCES IN FILE CA (1907 TO DATE)
.1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L9 ANSWER 11 OF 12 REGISTRY COPYRIGHT 2005 ACS on STN
RN 209669-43-2 REGISTRY ✓
ED Entered STN: 09 Aug 1998

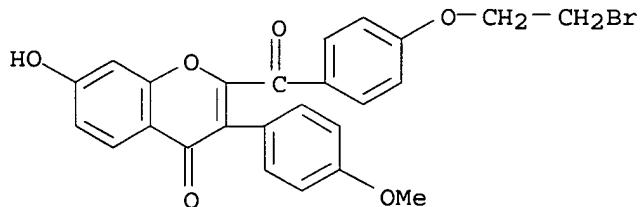
CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-methoxyphenyl)-2-[4-[2-(1-piperidinyl)ethoxy]benzoyl]-, hydrochloride (9CI) (CA INDEX NAME)
 OTHER NAMES:
 CN CHF 3290.01
 MF C30 H29 N O6 . Cl H
 SR CA
 LC STN Files: CA, CAPLUS
 CRN (791569-53-4)



● HCl

1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L9 ANSWER 12 OF 12 REGISTRY COPYRIGHT 2005 ACS on STN
 RN 209624-98-6 REGISTRY ✓
 ED Entered STN: 06 Aug 1998 ✓
 CN 4H-1-Benzopyran-4-one, 2-[4-(2-bromoethoxy)benzoyl]-7-hydroxy-3-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C25 H19 Br O6
 SR CA
 LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

| | | | |
|--|------------|---------|--|
| => fil caplus | | | |
| COST IN U.S. DOLLARS | SINCE FILE | TOTAL | |
| | ENTRY | SESSION | |
| FULL ESTIMATED COST | 183.41 | 233.80 | |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE | TOTAL | |
| | ENTRY | SESSION | |
| CA SUBSCRIBER PRICE | 0.00 | -9.49 | |

FILE 'CAPLUS' ENTERED AT 14:23:58 ON 02 APR 2005
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 PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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FILE COVERS 1907 - 2 Apr 2005 VOL 142 ISS 15
FILE LAST UPDATED: 1 Apr 2005 (20050401/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 19
L10 2 L9

=> d 1-2 fbib abs fhitstr

L10 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:466702 CAPLUS
DN 141:38528
TI Preparation of 2-benzoylchromone derivatives as inhibitors of the tyrosine kinase
IN Mujica-Fernaud, Teresa; Buchholz, Herwig; Carola, Christophe; Sirrenberg, Christian; Rautenberg, Wilfried
PA Merck Patent G.m.b.H., Germany
SO Ger. Offen., 22 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|------|----------|------------------|------------|
| DE 10256174 | A1 | 20040609 | DE 2002-10256174 | 20021202 |
| EP 1426378 | A1 | 20040609 | EP 2003-25849 | 20031111 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK | | | DE 2002-10256174 | A 20021202 |
| US 2004176440 | A1 | 20040909 | US 2003-725349 | 20031202 |
| | | | DE 2002-10256174 | A 20021202 |

OS CASREACT 141:38528; MARPAT 141:38528
GI

Arg

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB New compds. I [R = OH, OA, OPh, Ar, OC(:O)A, SO3H, SO3A, OSO3H, OSO3A, OSO2A, SO2A, halogen (F, Cl, I, Br), CO2H, CO2A, CONH2, NSO2A, COA, CHO, SO2NH2; RR = OCH2O, OCH2CH2O; A = (un)branched C1-10-alkyl, C1-10-fluoroalkyl; Ar = (un)substituted Ph; X = OH; XX = OCH2O, OCH2CH2O; n = 1 - 4; m = 1 - 5], their pharmaceutically acceptable derivs., solvates and stereoisomers, are inhibitors of the tyrosine kinase and can for the treatment by tumors, to the neuroprotection and for the protection of the stress proteins of the skin is used. The procedure for the preparation of I is characterized by: (a) hydroxyacetophenones II are cyclized with AOC(:O)C(:O)OA (A = C1-6-alkyl) to chromones III ; (b) hydrolysis of III to acid IV; (c) chlorination to acid chloride V ; (d) Friedel-Crafts acylation of PhRm. Thus, 5-Hydroxy-2-(2,4-dihydroxybenzoyl)chromone (VI) was prepared from 2,6-dihydroxyacetophenone via cyclocondensation with (EtO2C)2, hydrolysis with aqueous HCl in MeCO2H, chlorination with with

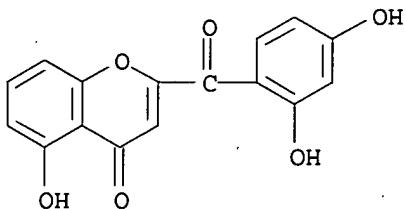
· ·(COCl)₂ in CH₂Cl₂ containing catalytic DMF, then Friedel-Crafts acylation of resorcinol in THF containing AlCl₃. Several drug dosage formulations are presented.

IT 700818-24-2P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 2-benzoylchromone derivs. as inhibitors of the tyrosine kinase)

RN 700818-24-2 CAPLUS

CN 4H-1-Benzopyran-4-one, 2-(2,4-dihydroxybenzoyl)-5-hydroxy- (9CI) (CA INDEX NAME)



L10 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1998:485049 CAPLUS

DN 129:95354

TI Preparation and formulation of isoflavone derivatives for the prophylaxis and treatment of osteoporosis

IN Chiesi, Paolo; Ventura, Paolo; Servadio, Vittorino; Delcanale, Maurizio; Amari, Gabriele; Armani, Elisabetta; Civelli, Maurizio; Giossi, Massimo; Galbiatti, Elisabetta

PA Chiesi Farmaceutici S.P.A., Italy

SO PCT Int. Appl., 22 pp.

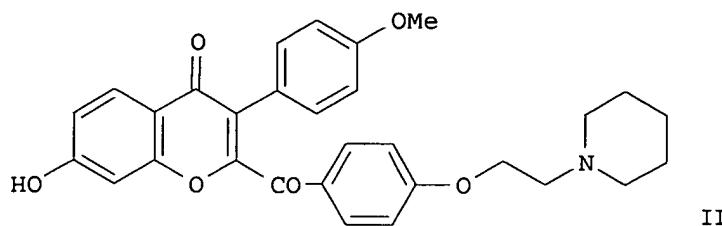
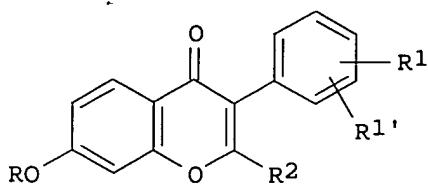
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|----|---|-----------|----------|-----------------|------------|
| PI | WO 9829403 | A1 | 19980709 | WO 1998-EPI1 | 19980101 |
| | W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG | | | IT 1997-MI3 | A 19970103 |
| | AU 9862066 | A1 | 19980731 | AU 1998-62066 | 19980101 |
| | | | | IT 1997-MI3 | A 19970103 |
| | | | | WO 1998-EPI1 | W 19980101 |
| | EP 954520 | A1 | 19991110 | EP 1998-904026 | 19980102 |
| | EP 954520 | B1 | 20020410 | | |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO | | | IT 1997-MI3 | A 19970103 |
| | | | | WO 1998-EPI1 | W 19980101 |
| | AT 215941 | E | 20020415 | AT 1998-904026 | 19980102 |
| | | | | IT 1997-MI3 | A 19970103 |
| | | | | WO 1998-EPI1 | W 19980101 |
| | ES 2175661 | T3 | 20021116 | ES 1998-904026 | 19980102 |
| | | | | IT 1997-MI3 | A 19970103 |
| OS | MARPAT | 129:95354 | | | |
| GI | | | | | |



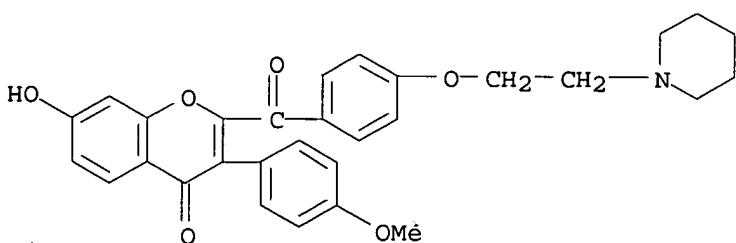
AB Isoflavones I [R = H, alkyl; R1 = H, OH, CF₃, OCF₃, halogen, alkyl, cycloalkyl, alkoxy; R1' = H, OH, halogen, alkyl, alkoxy; R2 = substituted benzoyl] were prepared for the prophylaxis and treatment of osteoporosis. Thus, isoflavone II.HCl, i.e. CHF 3290.01, was prepared starting from 4-MeOC₆H₄CH₂CO₂H, ClCOCO₂Et, PhO(CH₂)₂Br, and piperidine. The prepared compds. showed good activity in inhibiting bone resorption.

IT 209669-43-2P, CHF 3290.01

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation and formulation of isoflavone derivs. for the prophylaxis and treatment of osteoporosis)

RN 209669-43-2 CAPLUS

CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-methoxyphenyl)-2-[4-[2-(1-piperidinyl)ethoxy]benzoyl]-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RE.CNT 4

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT